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A PROGRAM FOR CALCULATING RADIATION FLOW AND HYDRODYNAMIC MOTION

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PREFACE

An important tool in weapon effects research is the numerical integration of the differential equations of motion for high temperature, high pressure gases. Computer programs which describe hydrodynamic motion and which can accommodate radiation transport have been helpful in describing blast effects, fireball growth, high explosive detonation waves, shock tube experiments, bubble expansions, radiation blow-off phenomena, thermal radiation phenomena, high altitude effects, and underground explosion initial phases.

Such programs have existed at RAND in various but increasing degrees of sophistication for the past 14 years. Many reports on blast waves, fireballs, etc., have presented results of such calculations. Currently, several other organizations use similar programs, but many more would enjoy the capability if such a code were generally available and easily applied.

This report attempts to answer a portion of that need by describing in detail a program designed for ease of application to a wide variety of problems. This program has evolved from earlier versions (by Brode), and is the product of the present authors' efforts over the past three years. Simplicity and generality are often mutually exclusive objectives. The compromises made in this computer program have tended to favor generality rather than simplicity on the supposition that it is easier for a user to simplify by dropping subroutines and unwanted features than to invent new routines in order to handle each new problem.

SUMMARY

This report contains a numerical program for solving hydrodynamic flow and radiation transport problems in the diffusion and grey-body approximations. The program is appropriate to the solution of explosion and shock wave problems, and to the study of high explosive or nuclear fireballs, hot gas dynamics, deflagrations and detonations, bubble phenomena, shock tube flows, and can be adapted to a host of other dynamics problems. It is restricted to plane, cylindrical, or spherical symmetry.

The report offers (1) a description of the assumed physical model, (2) a rationale for the difference equations and integration techniques used in the mathematical formulation, (3) a complete set of flow diagrams for the program and its subroutines, (4) a listing of the code, (5) two illustrative example calculations for hydrodynamics and for radiation flow, and (6) helpful hints for checking and running versions of the program.

I. INTRODUCTION

This is a world full of dynamics and transient phenomena, and our efforts to cope with and to better understand the physical forces and reactions associated with some of the high pressure, high temperature features have become both extensive and intensive. We search for theories to describe such widely differing time-dependent processes as occur in atmospheric re-entry of space vehicles or ballistic missiles, in nuclear explosions, stellar energetics, or lightning strokes. We look for rather precise descriptions for the dynamic properties of many such problems, even where the situation calls for coupled radiation and hydrodynamic flow treatment. In the absence of adequate analytic solutions, numerical procedures have grown to such sophistication as to be able to accommodate much of the physics involved and to include both greater realism and detail in treating boundary conditions, material properties, and geometrical factors. It is now practical to solve a wide variety of radiation and hydrodynamic flow problems by means of computer programs for numerical integration of differential formulations.

The object of this memorandum is to describe in detail one such numerical program. The program is capable of calculating in one space dimension (spherical, cylindrical, or plane symmetry) hydrodynamic motions including shocks. Radiation diffusion, grey-body or other radiation losses, and energy sinks or sources are simultaneously calculable with this code.

With such a program, calculations can be run which provide a reasonable approximation to the blast and thermal phenomena from nuclear or high explosive detonations. It can compute the responses of simple targets to blast and/or thermal radiation loads. It can predict some deep underground or underwater explosion phenomena, and can be used for transient blow-off and ablation descriptions. The program has been used to investigate shock flows down tunnels, the dynamics of lightning strokes, shock interactions, explosive dynamics in cavities, in space, and in a variety of materials and environments. In addition, shock and radiation flow characteristics can be studied

in reflection or transmission normal to interfaces - between air and water, between water and soil, or between various metals and/or other solids (treated as compressible fluids).

The general mechanisms for integrating the partial differential equations that govern the phenomena of radiation diffusion and hydrodynamic motions are approximately the same for all these types of investigations. The chief differences lie in the fixing of different initial and boundary conditions and in finding appropriate equations of state and opacities for the materials involved. Many of these latter problems have been minimized in the present program, and much of the pain and special programming usually required to set up a new problem can be avoided. The provision for simplified selection of output variables and display of results also makes it easier to get the most out of each problem.

However, the basic computational methods are similar to those of previous codes developed by one of us (Brode).

II. PHYSICAL ASSUMPTIONS AND MATHEMATICAL FORMULATION

A description of the dynamics of an explosion can be obtained from the solution of a set of nonlinear, partial differential equations which represent the conservation of mass, momentum, and energy in some symmetry. These conservation laws may be expressed mathematically in several ways, but are generally formulated in terms of either Eulerian or Lagrangian coordinates. The Eulerian form is an expression of the conservation laws as viewed from coordinate systems fixed in space, and the Lagrangian form is an expression of the same conservations in terms of a fixed set of masses or gas particles. A solution in the Eulerian case may represent the history of a blast wave at a fixed point, while in a Lagrangian system a solution may describe the experience of each particle (or an initially identified volume or mass of gas) as it moves about. Lagrangian (i.e., mass) coordinates are used in the present program.

Most of the currently useful methods for obtaining numerical solutions to problems in hydrodynamics (with or without radiation flow) employ a finite difference technique in which the motions are followed from some initial time to subsequent times through a series of finite time increments and over a set of discrete mass or space differential elements. The equations that govern this iterative integration procedure approximate the differential equations of flow and are called difference equations.

DIFFERENTIAL EQUATIONS

In terms of the variables explicitly treated in this program, expression of the conservation of mass takes the following differential form:

$$\frac{1}{\rho} = V = \frac{1}{3}\frac{\partial R^3}{\partial m} \quad \text{(spherical)}$$

$$= \frac{1}{2}\frac{\partial R^2}{\partial m} \quad \text{(cylindrical)} \qquad (1)$$

$$= \frac{\partial R}{\partial m} \quad \text{(plane)}$$

$$= \frac{1}{\delta} \frac{\partial R^{\delta}}{\partial m}, \qquad \delta = 1,2,3 \tag{1}$$

in which ρ represents density (V, specific volume), R a radius or spatial dimension, and m the mass.

It is understood that unit length is included in the volume of cylindrical symmetry, and unit area is included in the volume for plane geometry. The mass (m) is defined as the mass per steradian (Mass/4π) in spherical symmetry ($m = \int_o^r \rho r^2 dr$), while m is mass per radian per unit length (Mass/$2\pi\ell$) in cylindrical symmetry ($m = \int_o^r \rho r dr$), and is mass per unit area (Mass/ℓ^2) in plane symmetry ($m = \int_1^r \rho dx$).

The conservation of momentum in differential form appears as

$$\frac{\partial u}{\partial t} = - R^{\delta-1} \frac{\partial}{\partial m} (P+Q), \tag{2}$$

in which u is a particle or gas velocity, P represents pressure, Q is the artificial viscosity pressure, and t represents the time. The artificial viscosity is a convenience first introduced by Von Neumann and Richtmyer[1] for numerical treatment of shock waves. Its effect is to diffuse a shock front and thus avoid the paradoxical situation of discontinuities or sharp shock fronts running through discrete mass elements. A discontinuity in hydrodynamic parameters requires special treatment in finite difference numerical schemes in order to avoid extreme oscillations and instabilities. The artificial viscosity not only avoids special routines, but automatically accommodates all shocks, even multiple shocks wherever and whenever they occur. At the same time, with some care in selection of problem parameters such as zone size and artificial viscosity amplitudes, the spread of shocks can be held to a practical minimum and so not degrade the accuracy of results.

The artificial viscosity form originally considered (in plane geometry) by Von Neumann and Richtmyer was

$$Q = - \frac{(C\Delta m)^2}{V} \frac{\partial V}{\partial t} \left| \frac{\partial V}{\partial t} \right| , \qquad (3)$$

in which C is an arbitrary constant, dimensionless, and of value near unity. As this form indicates, for compressions (i.e., when $\partial V/\partial t$ is negative), a positive viscous pressure is generated, which has a magnitude proportional to the square of the rate of compression and the square of a mass element Δm.

Restricting viscous contributions to compressions only leads to a modified form[2]

$$Q = - \frac{(C\Delta m)^2}{2VR^{2(\delta-1)}} \frac{\partial V}{\partial t} \left[\frac{\partial V}{\partial t} - \left| \frac{\partial V}{\partial t} \right| \right] , \qquad (4)$$

in which we have included a dimensional factor to maintain C as dimensionless in cylindrical and spherical systems.

For weak shocks, this quadratic form tends to generate serious oscillations behind a shock front. A linear viscosity addition may aid in damping these oscillations. An appropriate linear form is similar:

$$Q' = - \frac{C'\Delta m}{2VR^{\delta-1}} \left[\frac{\partial V}{\partial t} - \left| \frac{\partial V}{\partial t} \right| \right] . \qquad (5)$$

A statement of the energy balance in differential form reflects the second law of thermodynamics

$$\frac{\partial E}{\partial t} + P \frac{\partial V}{\partial t} = - Q \frac{\partial V}{\partial t} - D - \frac{\partial L}{\partial m} , \qquad (6)$$

where the terms on the left represent an adiabatic relation between rates of change of internal energy (E) and the rate at which compressional work is done. The right hand side includes the dissipative viscosity term which provides the necessary entropy change in shocks. The D-term symbolizes a depletion rate, or (for negative values) an energy input rate.

The final term $(\partial L/\partial m)$, a luminosity gradient, represents the flow of energy in the diffusion limit. The luminosity itself is defined as the areal flux per unit angle, where the area is $R^{(\delta-1)}$ and the black body flux is $-(c\lambda/3)(\partial aT^4/\partial R)/\rho$. Thus, one may define the luminosity as

$$L = -(R^{2(\delta-1)}/k)\ (\partial T^4/\partial m), \qquad (7)$$

in which the Rosseland mean free path (λ) has been replaced by $3V/ack$, a is the radiation constant (see p. 9), and Eq. (1) has been used. The quantity k is related to the usual Rosseland mean opacity (K_R) by $k = 3K_R/ac$, and c is the velocity of light.*

In addition, it is necessary to describe the thermodynamic properties of the material, i.e., some constitutive relation between specific internal energy, pressure, and density for hydrodynamics. Radiation problems also require that an opacity (k) and temperature (T) be defined and related to the other thermodynamic variables. These equation of state functions can be expressed in various forms, but the basic form employed in this program expresses energy, pressure, and opacity as functions of temperature and specific volume (or density), i.e., $E(T,V)$, $P(T,V)$, $k(T,V)$.

DIFFERENCE EQUATIONS

Figure 1 denotes the particular choice of notation and concentration of variables at mass points and time points. In the particular system represented in Fig. 1 the mass is identified with the half points in the "j" variables, the time is centered at the half points in the "n" variable, and the various quantities such as the velocities, radii, specific volumes, pressures, and energies are identified at the times and mass points indicated in the diagram. With such an identification it is possible to translate the differential equations into difference equations which largely deal with centered quantities. That is, each difference equation is balanced about the same time point and the same mass point in order to avoid first order numerical errors in the approximation of differentials by finite differences. A common procedure is to begin, as in Eqs. (8-13), to

*For some physical problems it is important to note that this form does not account for retardation, and energy may transport faster than the speed of light.

develop at time n + 1 a new velocity and then to find a new radius for each j point. From the new radii one can define a new density or specific volume, and from the change in density, an artificial viscosity at the new time. In these equations subscripts (j or $j\pm\frac{1}{2}$) and superscripts (n, $n+\frac{1}{2}$, or n+1) indicate definitions of each particular quantity at those discrete times and masses.

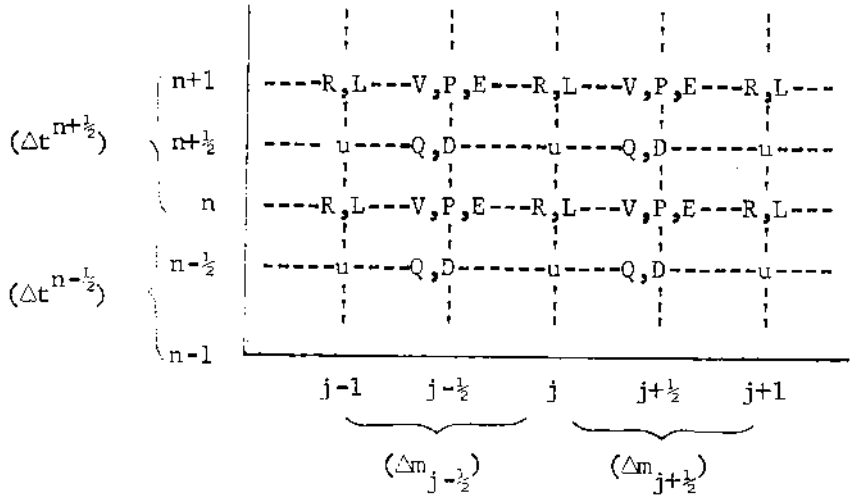

FIG. 1--Lagrangian difference grid for numerical calculation

First:

$$u_j^{n+\frac{1}{2}} = u_j^{n-\frac{1}{2}} - \frac{\Delta t^n}{\Delta m_j} (R_j^n)^{\delta-1} \left[P_{j+\frac{1}{2}}^n - P_{j-\frac{1}{2}}^n + Q_{j+\frac{1}{2}}^{n-\frac{1}{2}} - Q_{j-\frac{1}{2}}^{n-\frac{1}{2}} \right], \qquad (8)$$

in which

$$\Delta m_j = \tfrac{1}{2} \Delta m_{j+\frac{1}{2}} + \tfrac{1}{2} \Delta m_{j-\frac{1}{2}}, \qquad (9)$$

and

$$\Delta t^n = \tfrac{1}{2} \Delta t^{n+\frac{1}{2}} + \tfrac{1}{2} \Delta t^{n-\frac{1}{2}}. \qquad (10)$$

Then

$$R_j^{n+1} = R_j^n + u_j^{n+\frac{1}{2}} \Delta t^{n+\frac{1}{2}}, \qquad (11)$$

and

$$V_{j-\frac{1}{2}}^{n+1} = \frac{(R_j^{n+1})^\delta - (R_{j-1}^{n+1})^\delta}{\delta \Delta m_{j-\frac{1}{2}}} = \frac{1}{\rho_{j-\frac{1}{2}}^{n+1}}. \qquad (12)$$

The artificial viscosity becomes

$$Q_{j-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{C_1(\Delta m_{j-\frac{1}{2}})^2(V_{j-\frac{1}{2}}^{n+1} - V_{j-\frac{1}{2}}^{n})^2}{(V_{j-\frac{1}{2}}^{n+1} + V_{j-\frac{1}{2}}^{n})(\Delta t^{n+\frac{1}{2}})^2 \left\langle \frac{R_j^{n+1} + R_{j-1}^{n+1}}{2} \right\rangle^{2(\delta-1)}}$$

$$+ \frac{C_2\, \Delta m_{j-\frac{1}{2}} \left| V_{j-\frac{1}{2}}^{n+1} - V_{j-\frac{1}{2}}^{n} \right|}{(V_{j-\frac{1}{2}}^{n+1} + V_{j-\frac{1}{2}}^{n})(\Delta t^{n+\frac{1}{2}}) \left\langle \frac{R_j^{n+1} + R_{j-1}^{n+1}}{2} \right\rangle^{\delta-1}} , \qquad (13)$$

for $V^{n+1} < V^n$, and

$$Q_{j-\frac{1}{2}}^{n+\frac{1}{2}} = 0 \qquad \text{for} \qquad V^{n+1} \geq V^n .$$

It is in the energy equation alone that radiation enters (except radiation pressure which can contribute to the momentum only at exhalted temperatures). For hydrodynamics only, the energy equation can be written as

$$E_{j-\frac{1}{2}}^{n+1} = E_{j-\frac{1}{2}}^{n} + (\tfrac{1}{2}P_{j-\frac{1}{2}}^{n+1} + \tfrac{1}{2}P_{j-\frac{1}{2}}^{n} + Q_{j-\frac{1}{2}}^{n+\frac{1}{2}})(V_{j-\frac{1}{2}}^{n} - V_{j-\frac{1}{2}}^{n+1}) . \qquad (14)$$

RADIATION DIFFUSION

When radiation diffusion is included, the luminosity as defined in Eq. (7) becomes in difference form

$$L_j^n = \frac{(R_j^n)^{2(\delta-1)}\left[(T_{j-\frac{1}{2}}^{n})^4 - (T_{j+\frac{1}{2}}^{n})^4\right]}{(k\Delta m)_j^n} . \qquad (15)$$

The opacity is averaged with the mass increments and reduced by the factor ac/3 in which c is the speed of light and a is the radiation density constant (7.62×10^{-15} erg/cm^3/deg^4).

$$(k\Delta m)^n_j = \tfrac{1}{2}\Delta m_{j-\frac{1}{2}}\, k^n(T^n_j, V^n_{j-\frac{1}{2}}) + \tfrac{1}{2}\Delta m_{j+\frac{1}{2}} k^n(T^n_j, V^n_{j+\frac{1}{2}}) \ , \qquad (16)$$

$$k = \frac{3}{ac} K_R = \frac{3}{ac} \frac{V}{\lambda} \ .$$

The opacity is calculated for the material to the left of the point j for $k^n(T^n_j, V^n_{j-\frac{1}{2}})$ and for the material to the right of the point j for $k^n(T^n_j, V^n_{j+\frac{1}{2}})$. The temperature T^n_j is defined as $\left[\tfrac{1}{2}(T^n_{j+\frac{1}{2}})^4 + \tfrac{1}{2}(T^n_{j-\frac{1}{2}})^4\right]^{\frac{1}{4}}$. This procedure provides a reasonable opacity at interfaces between materials of very different opacity, and does not add undue complexity when the materials are the same.

EXPLICIT RADIATION DIFFUSION

For an explicit scheme of including radiation diffusion (one which has an explicit stability limitation to the size of time increment allowed), the energy equation becomes

$$E^{n+1}_{j-\frac{1}{2}} = E^n_{j-\frac{1}{2}} + (P^{n+\frac{1}{2}}_{j-\frac{1}{2}} + Q^{n+\frac{1}{2}}_{j-\frac{1}{2}})(V^n_{j-\frac{1}{2}} - V^{n+1}_{j-\frac{1}{2}}) + \frac{\Delta t^{n+\frac{1}{2}}}{\Delta m_{j-\frac{1}{2}}}(L^n_{j-1} - L^n_j) - D^{n+\frac{1}{2}}_{j-\frac{1}{2}} \ , \qquad (17)$$

in which $D^{n+\frac{1}{2}}_{j-\frac{1}{2}}$ is a source or sink term yet to be specified.

Some iterative converging solution of Eq. (17) is necessary in which values of $P^{n+\frac{1}{2}}_{j-\frac{1}{2}} = (P^{n+1}_{j-\frac{1}{2}} + P^n_{j-\frac{1}{2}})/2$ and E^{n+1} are sought which satisfy both Eq. (17) and the equation of state E(P,V) or E(T,V), P(T,V). In this explicit form, such iterative convergence is limited to the two variables $E^{n+1}_{j-\frac{1}{2}}$ and $P^{n+1}_{j-\frac{1}{2}}$, all other quantities being of fixed value for that step. When a new energy and pressure have been derived, a new temperature $(T^{n+1}_{j-\frac{1}{2}})$ also exists, and so, ultimately, new opacities and luminosities can be computed for the

next time cycle.

The set of equations (Eqs. 12-17) together with the equations of state and opacities form a set of equations whose solution for "new" values of each variable at all of the mass points can be directly obtained by successively evaluating each equation beginning with j = 0 and proceeding through the maximum j-point, or through all the "active" zones.

IMPLICIT RADIATION DIFFUSION

The implicit diffusion treatment is a form in which the luminosities are treated as centered at the midpoint in time $(n+\frac{1}{2})$ rather than taken at the previous time (n) as in the above explicit form in Eq. (17). Thus the form of the energy equation becomes

$$E^{n+1}_{j-\frac{1}{2}} = E^{n}_{j-\frac{1}{2}} + (\tfrac{1}{2}P^{n+1}_{j-\frac{1}{2}} + \tfrac{1}{2}P^{n}_{j-\frac{1}{2}} + Q^{n+\frac{1}{2}}_{j-\frac{1}{2}})(V^{n}_{j-\frac{1}{2}} - V^{n+1}_{j-\frac{1}{2}}) + \frac{\Delta t^{n+\frac{1}{2}}}{2\Delta m_{j-\frac{1}{2}}}(L^{n+1}_{j-1} + L^{n}_{j-1} - L^{n+1}_{j} - L^{n}_{j}) - D^{n+\frac{1}{2}}_{j-\frac{1}{2}} . \tag{18}$$

In this implicit form the variables to be simultaneously determined are now L^{n+1}_{j} and L^{n+1}_{j-1} in addition to $E^{n+1}_{j-\frac{1}{2}}$ and $P^{n+1}_{j-\frac{1}{2}}$. But these energy equation variables are no longer independent of other mass points as they were before, and it is now necessary to solve all of the energy (and equation of state and opacity) equations for all of the mass points simultaneously to arrive at new values. Although such a simultaneous "relaxation" of these equations avoids the restriction of an explicit stability limitation on the time step size permissible, it does add considerable computational complication and redundant numerical exercise to the problem, and so can increase the running time per time step several fold - in part negating the freedom to choose larger time intervals. The procedure consists of the evaluation of a set of forward-backward substitution coefficients, related to the proximity of variables to their proper values in a self consistent set of solutions, i.e., related to a measure of the relaxation in a

given time step.* In this process, the basic variables are taken as temperature (T) and luminosity (L).

Beginning with j = 1, the following quantities are computed:

$$\sum_{j-\frac{1}{2}}^{n+1} \equiv 2\Delta m_{j-\frac{1}{2}} \left[E^{n}_{j-\frac{1}{2}} - E^{n+1}_{j-\frac{1}{2}} \right. \tag{19}$$

$$\left. + \left(\frac{P^{n+1}_{j-\frac{1}{2}} + P^{n}_{j-\frac{1}{2}}}{2} + Q^{n+\frac{1}{2}}_{j-\frac{1}{2}} \right) \cdot \left(V^{n}_{j-\frac{1}{2}} - V^{n+1}_{j-\frac{1}{2}} \right) - D^{n+\frac{1}{2}}_{j-\frac{1}{2}} \right] ,$$

$$C^{n+1}_{j-\frac{1}{2}} \equiv 2\Delta m_{j-\frac{1}{2}} \left[\frac{\partial E^{n+1}_{j-\frac{1}{2}}}{\partial T^{n+1}_{j-\frac{1}{2}}} + \frac{\partial P^{n+1}_{j-\frac{1}{2}}}{\partial T^{n+1}_{j-\frac{1}{2}}} \left(\frac{V^{n+1}_{j-\frac{1}{2}} - V^{n}_{j-\frac{1}{2}}}{2} \right) \right] , \tag{20}$$

$$\frac{\partial E^{n}}{\partial T^{n}} \equiv \frac{E(T^{n}, V^{n}) - E^{n}\left[T^{n}(1+\epsilon), V^{n}\right]}{\epsilon T^{n}} , \text{ where typically } \epsilon \lesssim 10^{-4} \tag{21}$$

$$H^{n+1}_{j-\frac{1}{2}} \equiv C^{n+1}_{j-\frac{1}{2}} + \Delta t^{n+\frac{1}{2}} G^{n+1}_{j-1} , \tag{22}$$

$$K^{n+1}_{j-\frac{1}{2}} \equiv \left[\sum_{j-\frac{1}{2}}^{n+1} + \Delta t^{n+\frac{1}{2}} \left(L^{n+1}_{j-1} + L^{n}_{j-1} - L^{n+1}_{j} - L^{n}_{j} \right) \right] + \Delta t^{n+\frac{1}{2}} J^{n+1}_{j-1} , \tag{23}$$

in which $J^{n+1}_{o} = G^{n+1}_{o} = 0$ (for spherical or cylindrical symmetry);

*This particular forward-backward substitution scheme, coupled with a Newton's method for projecting new values, was suggested by R.E. LeLevier and has been used successfully in earlier similar programs.

$$\sigma_j^{n+1} \equiv (R_j^{n+1})^{2(\delta-1)} \left[(T_{j-\frac{1}{2}}^{n+1})^4 - (T_{j+\frac{1}{2}}^{n+1})^4 \right] - (k\Delta m)_j^{n+1} L_j^{n+1} , \qquad (24)$$

$$a_{j+\frac{1}{2}}^{n+1} \equiv 4(R_j^{n+1})^{2(\delta-1)} (T_{j+\frac{1}{2}}^{n+1})^3 + L_j^{n+1} \frac{\partial (k\Delta m)_j^{n+1}}{\partial T_{j+\frac{1}{2}}^{n+1}} , \qquad (25)$$

$$b_{j-\frac{1}{2}}^{n+1} \equiv 4(R_j^{n+1})^{2(\delta-1)} (T_{j-\frac{1}{2}}^{n+1})^3 - L_j^{n+1} \frac{\partial (k\Delta m)_j^{n+1}}{\partial T_{j-\frac{1}{2}}^{n+1}} , \qquad (26)$$

$$G_j^{n+1} \equiv \frac{a_{j+\frac{1}{2}}^{n+1} H_{j-\frac{1}{2}}^{n+1}}{(k\Delta m)_j^{n+1} H_{j-\frac{1}{2}}^{n+1} + \Delta t^{n+\frac{1}{2}} b_{j-\frac{1}{2}}^{n+1}} , \qquad (27)$$

$$J_j^{n+1} \equiv \frac{H_{j-\frac{1}{2}}^{n+1} \sigma_j^{n+1} + b_{j-\frac{1}{2}}^{n+1} K_{j-\frac{1}{2}}^{n+1}}{(k\Delta m)_j^{n+1} H_{j-\frac{1}{2}}^{n+1} + \Delta t^{n+\frac{1}{2}} b_{j-\frac{1}{2}}^{n+1}} . \qquad (28)$$

These coefficients are successively evaluated for each increasing integer value of j (at each mass point) until the next j is at a point beyond the sensible diffusion front where temperature changes from ambient are negligible. This zone is designated as the turn-around point (j*) where conditions are such that $T_{j^*-\frac{1}{2}}^n > Z_1$ but $T_{j^*+\frac{1}{2}}^n < Z_1$. When there is no temperature gradient, the luminosity must be zero, so that $L_{j^*+1} \approx 0$, providing $T_{j+\frac{1}{2}} < Z_1$ for all $j > j^*$, Z_1 being small.

The procedure then is to compute changes in temperature and luminosity (using the foregoing coefficients) beginning at j* and working back to j = 0.

The temperature at $j^* + \frac{1}{2}$ on the (i + 1)st iteration is first calculated as

$$ {}^{i+1}T_{j^*+\frac{1}{2}}^{n+1} = {}^{i}T_{j^*+\frac{1}{2}}^{n+1} + \delta T_{j^*+\frac{1}{2}} , \tag{29} $$

where

$$ \delta T_{j^*+\frac{1}{2}} = K_{j^*+\frac{1}{2}}^{n+1} \Big/ H_{j^*+\frac{1}{2}}^{n+1} . \tag{30} $$

Then beginning with $j = j^*$, successive evaluations go as

$$ \delta L_j = - G_j^{n+1} \, \delta T_{j+\frac{1}{2}} + J_j^{n+1} , \tag{31} $$

$$ {}^{i+1}L_j^{n+1} = {}^{i}L_j^{n+1} + \delta L_j , \tag{32} $$

$$ \delta T_{j-\frac{1}{2}} = (-\Delta t^{n+\frac{1}{2}} \, \delta L_j + K_{j-\frac{1}{2}}^{n+1}) / H_{j-\frac{1}{2}}^{n+1} , \tag{33} $$

reducing j each time until j = 1. "Relaxation" or convergence is determined by testing each $\delta T/T$ or $\delta L/L$ against an arbitrary small constant and entering another iteration loop to recompute the coefficients and another set of δT and δL as long as any one δT or δL exceeds the chosen test constant.

ADDED MASS

Since interests in explosion problems encompass phenomena occuring both very close to the explosive (in a small mass and volume) and very far from the source (with very large masses and volumes of air

intervening), it is frequently convenient to bring in more air mass during the calculation.

To expand the mass system without adding indefinitely to the number of mass points carried requires some mechanism for dropping or rather combining interior masses as new masses are added at a front. When zones are combined, special care should be taken to conserve energy, momentum and mass. In this program, one zone at a time (as needed) is added, and two zones elsewhere (in the interior) are combined in order to keep constant the number of zones carried in the calculation. Because of the form of the artificial viscosity, sudden discontinuities in mass element size can create spurious signals as shocks cross them. For this reason, some care must be exercised in deciding when and where zones may be combined. Generally, zones are selected to be combined where motions and pressure or temperature gradients are least, i.e., in such a way as to retain essential problem detail while not unduly restricting the size of time steps dictated by stability requirements.

SOURCES, SINKS, AND DEPLETION

The single variable, D, appearing in the energy equations can be used to represent such physical features as can be expressed as energy losses or sources. Such source or sink energy rates may be included in some or all zones in the problem and may vary with time. The detonation of high explosive can be modeled by choosing this source term to represent the rate at which energy is released in detonations. With a finite spread to the detonation front, this source term becomes the product of the energy generated per unit mass of explosive (E_{CJ}), the detonation velocity (U_{CJ}), and the time increment ($\Delta t^{n+\frac{1}{2}}$), divided by the total spread of the detonation front appropriate to that dictated by the artificial viscosity, i.e.,

$$D_{j-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{-E_{CJ}\, U_{CJ}\, \Delta t^{n+\frac{1}{2}}}{S\, \Delta R_{j-\frac{1}{2}}} , \qquad (34)$$

where S is the number of zones of detonation front spread. Such a rate of energy increase would then be maintained in each zone until the total energy added equals the desired detonation energy, i.e., for a time equal to $S\Delta R/U_{CJ}$.

STABILITY REQUIREMENTS

Such finite difference methods as employed here are frequently subject to mathematical limitations which place upper bounds on the size of time increments that can be taken without the unstable growth of spurious signals from truncation or round-off error. The usual Courant Condition is simply a statement that time steps should be smaller than the time for a sound signal to propagate beyond the boundaries of adjacent zones (as in Fig. 2). Thus, $\Delta t < \Delta R/s$ for every zone, or $\Delta t < \left[\Delta R_{j-\frac{1}{2}}/s_{j-\frac{1}{2}}\right]_{min}$, in which s is the local sound speed. It is generally time consuming to calculate the sound speed at each zone when an approximate form which is quicker to compute will suffice to determine the maximum allowable time step within a reasonable accuracy. For an ideal gas, the sound speed squared is given by

$$s^2 = \gamma P/\rho = \gamma PV, \tag{35}$$

and the stability condition can be expressed as

$$\Delta t^2 \lesssim V(\Delta m)^2/(C_3 P\, R^{2(\delta-1)}), \tag{36}$$

in which we have substituted $\Delta R = V\,\Delta m/R^{(\delta-1)}$ and C_3 is the maximum value of γ to be encountered and depends on the materials used and their equations of state. For ideal gases, a value of 5/3 is a maximum, and lesser values are larger than unity always, so that using 5/3 for C_3 could keep Δt smaller than necessary by no more than 23%. For the dense gases of detonation products before expansion, or for fluids such as water, or for solids at high temperatures and densities the effective maximum γ can exceed 5/3, and the constant C_3 should be chosen with that in mind.

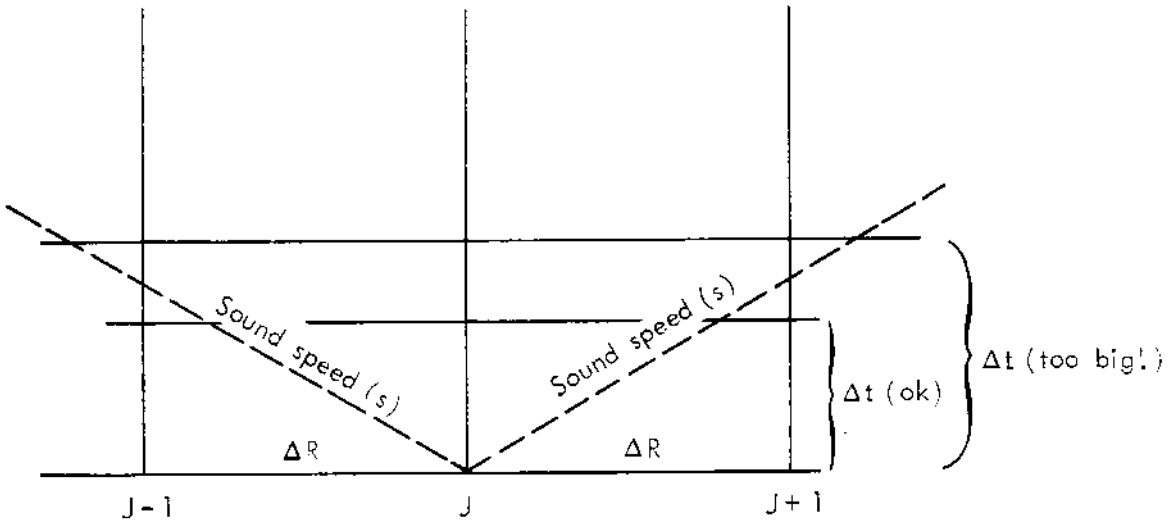

Fig.2—Courant stability condition

In shock fronts or compression regions, the presence of a quadratic artificial viscosity changes the nature of the linearized differential equations from one which characterizes a wave equation to one of a diffusion type. Consequently, in such shock regions another difference equation stability condition exists, a diffusion stability limit. An approximate derivation of the viscosity stability condition comes from the momentum conservation equation (Eq. 2), with the assumption that the artificial viscosity pressure (Q) dominates the usual thermodynamic pressure (P). In that case,

$$\frac{\partial u}{\partial t} \simeq - R^{\delta-1} \frac{\partial Q}{\partial m} . \tag{37}$$

In regions of compression, the quadratic form of the artificial viscosity has been taken as

$$Q = \frac{C_1 (\Delta m)^2}{V R^{2(\delta-1)}} \left(\frac{\partial V}{\partial t}\right)^2 + \frac{C_2 \Delta m}{V R^{\delta-1}} \frac{\partial V}{\partial t} . \tag{38}$$

But differentiating the conservation of mass equation (Eq. 1), and substituting for $\partial V/\partial t$ leads to

$$Q = \frac{C_1 (\Delta m)^2}{V R^{2(\delta-1)}} \left(\frac{\partial R^{\delta-1} u}{\partial m}\right)^2 + \frac{C_2 \Delta m}{V R^{\delta-1}} \frac{\partial (R^{\delta-1} u)}{\partial m} . \tag{39}$$

With this form and from

$$\frac{V}{R^{\delta-1}} = \frac{\partial R}{\partial m} , \tag{40}$$

the momentum equation in a shock (Eq. 37) becomes approximately

$$\frac{\partial u}{\partial t} \simeq - C_1 (\Delta m)^2 V \frac{\partial}{\partial R} \left[\frac{V}{R^{2(\delta-1)}} \left(\frac{\partial u}{\partial R}\right)^2 \right] - C_2 \Delta m \frac{V \partial}{\partial R} \left[\frac{1}{R^{\delta-1}} \frac{\partial u}{\partial R} + \frac{(\delta-1)}{R^{\delta}} u \right] , \tag{41}$$

and ignoring geometric divergence terms which occur in cylindrical or spherical symmetry (valid as long as shock front dimensions are small compared to radii or other problem dimensions) this equality becomes

$$\frac{\partial u}{\partial t} \simeq - \frac{2C_1(\Delta m)^2 V^2}{R^{2(\delta-1)}} \frac{\partial u}{\partial R} \frac{\partial^2 u}{\partial R^2} - \frac{V C_2 \Delta m}{R^{\delta-1}} \frac{\partial^2 u}{\partial R^2} . \tag{42}$$

In shock regions, derivatives such as $\partial u/\partial t$ or $\partial^2 u/\partial R^2$ are large; i.e., rapid velocity changes and velocity gradient changes are taking place relative to changes in other parameters, so that to some approximation this equation appears as a diffusion form

$$\frac{\partial u}{\partial t} \simeq K \frac{\partial^2 u}{\partial R^2} ,$$

where

$$K = \frac{V\Delta m}{R^{\delta-1}} \left[C_2 + 2C_1 \frac{V\Delta m}{R^{\delta-1}} \left| \frac{\partial u}{\partial R} \right| \right] , \quad (\text{for } \frac{\partial u}{\partial R} < 0), \tag{43}$$

which is considered nearly constant or slowly varying in the region of interest. Since we have not chosen to define the artificial viscosity at the midpoint between the new and the old velocity, but rather have defined it at the old velocity time $(n-\frac{1}{2})$, this diffusion differential form (Eq. 43) translates into a corresponding difference equation which uses velocities at adjacent mass points and at the old time $(n-\frac{1}{2})$ to extrapolate to a new velocity at time $n+\frac{1}{2}$

$$u_j^{n+\frac{1}{2}} \simeq u_j^{n-\frac{1}{2}} - K \frac{\Delta t^n}{(\Delta R_j^n)^2} (u_{j+1}^{n-\frac{1}{2}} - 2u_j^{n-\frac{1}{2}} + u_{j-1}^{n-\frac{1}{2}}) . \tag{44}$$

By considering the growth of perturbations in the new velocity (see Von Neumann and Richtmyer, Ref. 1, p. 236), it becomes clear that stability for such a forward-difference scheme has an explicit stability condition which is

$$\Delta t \leq \frac{(\Delta R)^2}{2K}\Big]_{\min} = \left.\frac{(\Delta R)^2 R^{\delta-1}}{2\left[C_2 + 2C_1 \frac{V\Delta m}{R^{\delta-1}} \left|\frac{\partial u}{\partial R}\right|\right] V\Delta m}\right]_{\min}$$

or (45)

$$\frac{2\Delta t}{\Delta R}\left[C_2 + 2C_1 \Delta R \left|\frac{\partial u}{\partial R}\right|\right]_{\max} \leq 1 .$$

But, again ignoring geometric divergence terms,

$$\frac{\partial u}{\partial R} = \frac{R^{\delta-1}}{V}\frac{\partial u}{\partial m} = \frac{R^{\delta-1}}{V}\left[\frac{1}{R^{\delta-1}}\frac{\partial V}{\partial t} - \frac{(\delta-1)u}{R}\right] \simeq \frac{1}{V}\frac{\partial V}{\partial t} \simeq \frac{V^{n+1}-V^n}{V^{n+\frac{1}{2}}\Delta t^{n+\frac{1}{2}}} , \tag{46}$$

so that

$$\left[\frac{2C_2\Delta t^{n+\frac{1}{2}}}{R_j^{n+\frac{1}{2}} - R_{j-1}^{n+\frac{1}{2}}} + 4C_1 \frac{\left|V_{j-\frac{1}{2}}^{n+1} - V_{j-\frac{1}{2}}^{n}\right|}{V_{j-\frac{1}{2}}^{n+\frac{1}{2}}}\right]_{\max} \leq 1 . \tag{47}$$

When the explicit form is used to compute radiation diffusion, a similar forward-difference stability condition applies, viz,

$$\Delta t < \frac{\Delta m^2}{2C''}\Big)_{\min} = \left.\frac{(k\Delta m)\left(\frac{\partial E}{\partial T}\right)\Delta m}{8T^3R^{2(\delta-1)}}\right]_{\min} . \tag{48}$$

Since for various regions and various reasons the implicit radiation diffusion routines are unable to converge on a realistic solution and are for practical purposes unstable beyond some reasonably small time steps, it is often necessary to arbitrarily limit the size of time steps to a value larger than but proportional to that allowed for explicit radiation. To make such a choice convenient, the program includes an explicit stability condition with a constant (C_5) which can be chosen as suitable for implicit radiation (e.g., equal to 2,3, or 4), but must be taken as unity for the explicit routines.

These three stability conditions are:

Courant:

$$\Omega^n \equiv \left[\frac{(\Delta t^{n+\frac{1}{2}})^2 (R_j^n)^{2(\delta-1)} P^n_{j-\frac{1}{2}} C_3}{V^n_{j-\frac{1}{2}} (\Delta m_{j-\frac{1}{2}})^2} \right]_{max} \leq 1 . \qquad (49)$$

Shock (artificial viscosity):

$$\Lambda^n \equiv \left[\frac{2C_2}{R_j^{n+\frac{1}{2}} - R_{j-1}^{n+\frac{1}{2}}} + C_4 \frac{(V^{n+1}_{j-\frac{1}{2}} - V^n_{j-\frac{1}{2}})}{V^{n+\frac{1}{2}}_{j-\frac{1}{2}} \Delta t^{n-\frac{1}{2}}} \right]_{max} \Delta t^{n+\frac{1}{2}} \leq 1, \qquad (50)$$

in which $C_4 \geq 4C_1$.

Radiation diffusion;

$$\Gamma^n \equiv \left[\frac{8(R_j^n)^{2(\delta-1)} (T_j^n)^3}{C_5 \Delta m_j (k\Delta m)^n_j \left(\frac{\partial E}{\partial T}\right)^n_{j-\frac{1}{2}}} \right]_{max} \Delta t^{n+\frac{1}{2}} \leq 1 . \qquad (51)$$

$C_5 = 1$ for explicit radiation.

$C_5 \geq 1$ for implicit (open choice).

III. HYDRODYNAMIC EXAMPLE

A simple test problem will facilitate the explanation of the essential features of this program. In any such code there are many arbitrary designations and notations which are easier demonstrated than explained. Hopefully, none of the empirical choices have significant influence on the results of any calculations in so far as the physical representation is concerned. Some of the parameters, such as choice of the number of zones or mass points, choice of zone sizes, or choices of convergence test criteria do affect the results when a choice becomes extreme or so coarse as to reduce accuracy. A few example calculations may help demonstrate both appropriate values for such constants as are required and the need or function of each input required.

As a simplest beginning, a plane shock wave generated by a constant pressure at one boundary will be demonstrated. Such a problem has a simple analytical solution, and the deviations from the correct solution that occur when we make various choices of parameters are easily identified. When the constant pressure is applied at the left-hand boundary of a volume of ideal gas, a shock of constant strength should move at constant speed to the right. The usual Hugoniot or shock conservation conditions relate the conditions behind a plane shock to those in front of it as follows:

$$\frac{u_s}{U} = 1 - \frac{\rho_o}{\rho_s} \quad \text{or} \quad \rho_o U = \rho_s (U - u_s) \ , \quad \text{(mass)} \ \ldots \qquad (52)$$

$$E_s - E_o = \frac{P_s + P_o}{2} \left(\frac{1}{\rho_o} - \frac{1}{\rho_s}\right) \ , \quad \text{(energy)} \ \ldots \qquad (53)$$

$$P_s - P_o = \rho_o \, u_s \, U \ , \quad \text{(momentum)} \ldots \qquad (54)$$

in which subscripts "s" refer to shock quantities, subscripts "o" refer to ambient (pre-shock) values, U is the shock velocity, u the particle velocity, ρ the density, P the pressure, and E the internal energy. It has further been assumed that the pre-shock gas velocity is zero.

If one defines an "effective gamma" by the relation $E = P/\rho(\gamma-1)$, i.e., $\gamma \equiv 1 + P/E\rho$, and eliminates internal energies from these Hugoniot expressions, then in place of the energy equation, one can write

$$\frac{\rho_s}{\rho_o} = \frac{\left(\frac{P_s}{P_o}\right)\cdot\left(\frac{\gamma_s + 1}{\gamma_s - 1}\right) + 1}{\frac{P_s}{P_o} + \left(\frac{\gamma_o + 1}{\gamma_o - 1}\right)} \quad . \tag{55}$$

Eliminating the shock velocity (U) from Eqs. (52) and (54), leads to an expression for the square of the peak particle velocity (u_s) in terms of density and pressure,

$$u_s^2 = \frac{(P_s - P_o)}{\rho_o}\left(1 - \frac{\rho_o}{\rho_s}\right), \qquad \ldots \tag{56}$$

and using Eq. (55) to eliminate density leads to

$$u_s^2 = \frac{2(P_s - P_o)}{\rho_o} \frac{\left[\frac{P_s}{P_o}\left(\frac{1}{\gamma_s-1}\right) - \frac{1}{\gamma_o-1}\right]}{\left[\frac{P_s}{P_o}\left(\frac{\gamma_s+1}{\gamma_s-1}\right) + 1\right]} \quad . \tag{57}$$

For an ideal gas ($\gamma_s = \gamma_o$), this expression reduces to

$$u_s^2 = \frac{2(P_s - P_o)^2}{[(\gamma+1)P_s + (\gamma-1)P_o]\rho_o} \quad . \tag{58}$$

Similarly, the square of the shock velocity becomes

$$U^2 = \frac{(\gamma+1)P_s+(\gamma-1)P_o}{2\rho_o} . \quad \ldots \quad (59)$$

With a value of γ equal to 7/5 (corresponding to an ideal diatomic molecule gas and appropriate for air at normal temperatures) these expressions reduce to the following:

$$U = \sqrt{\frac{6P_s+P_o}{5\rho_o}} , \quad \ldots \quad (60)$$

$$u_s = \frac{(P_s-P_o)}{\sqrt{\rho_o(6P_s+P_o)/5}} , \quad \ldots \quad (61)$$

and the density ratio becomes

$$\frac{\rho_s}{\rho_o} = \frac{6P_s+P_o}{P_s+6P_o} . \quad \ldots \quad (62)$$

The specific example used to illustrate the mechanics of running a hydrodynamics shock problem employs a suddenly applied, steady pressure at the left-hand boundary, and that pressure was chosen as one kilobar, or 10^9 dynes/cm^2. The ambient pressure into which the disturbance propagates is taken as that corresponding to an ambient density of 0.0011 gm/cm^3 and a temperature of 293°K in an ideal diatomic gas (γ = 1.4, R $\simeq$ 2.8777 x 10^{+6} dyne-cm/gm/$^\circ$K). The caloric equation of state becomes

$$P = (\gamma-1)\rho E = 0.4\rho E , \quad \ldots \quad (63)$$

and the thermal equation of state becomes

$$T = \frac{P}{\rho R} = \left(\frac{\gamma-1}{R}\right) E = 1.39 \times 10^{-7} E, \quad \ldots \quad (64)$$

with T in $^\circ$K and E in ergs/gm, P in dyne/cm^2 and ρ in gm/cm^3.

The value of the ambient pressure is approximately 0.927482 bars. The pre-shock energy is about 2.10791 x 10^9 ergs/gm. Thus, from the above relations (Eqs. 60-64) and the above pre-shock values and for a driving pressure of 10^9 dynes/cm^2, the pre- and post-shock values can be computed and used to check the performance of the numerical program. These values are listed in Table I below.

Table 1

SHOCK PARAMETERS FOR EXAMPLE CALCULATION

Symbol	Hydrodynamic Parameter	Pre-Shock	Post-Shock
P	Pressure(dyne/cm^2)	0.927482×10^6	10^9
ρ	Density(gm/cm^3)	1.1×10^{-3}	6.56173×10^{-3}
u	Particle velocity (cm/sec)	0	869,452
U	Shock velocity (cm/sec)	—	1,044,552
E	Energy(erg/gm)	2.10791×10^9	3.80999×10^{11}
T	Temperature($^\circ$K)	293.00	52,959

In this demonstration problem we have arbitrarily chosen thirty zones of one centimeter thickness into which the disturbance (shock) may propagate. The initial conditions in these zones, as well as in any zones to be added later, are the pre-shock conditions listed above.

The initial time step may be taken as anything less than that which the stability conditions stipulate, but too small an initial step may require many cycles to build up to a significant increment since the program limits increases in $\Delta t^{n+\frac{1}{2}}$ to $(9/8)\Delta t^{n-\frac{1}{2}}$. In cases of a suddenly applied load or an initially rapidly moving boundary, the stability conditions may not provide a correct limit on the first cycle. In any case, such failure is avoidable by insuring that the initial step is chosen as less than the time for a boundary to move across the next zone, and/or less than the time for a sound signal to cross that zone.

The acceleration of the left hand boundary on the first cycle is approximately

$$\frac{\delta u}{\Delta t} \simeq \frac{P_{-\frac{1}{2}} - P_{\frac{1}{2}}}{\Delta m_o} , \tag{65}$$

in which $\Delta m_j \equiv (\Delta m_{j+\frac{1}{2}} + \Delta m_{j-\frac{1}{2}})/2$ and $\Delta m_{-\frac{1}{2}} = 0$. The pressure, $P_{-\frac{1}{2}}$ is the boundary pressure of 10^9 dyne/cm^2, $P_{\frac{1}{2}}$ is the ambient pressure ($\sim 10^6$ dyne/cm^2), and a $\Delta m_{j+\frac{1}{2}} = \rho_{j+\frac{1}{2}} \Delta R_{j+\frac{1}{2}} = 1.1\text{x}10^{-3}$ gm/cm^2. Thus the velocity of the left boundary after the first time step is

$$u_o^{\frac{1}{2}} = \Delta t^o \frac{(P_{-\frac{1}{2}}^o - P_{\frac{1}{2}}^o)}{\Delta m_o} \simeq \Delta t^o \; 1.818\text{x}10^{12} (\text{cm/sec}) . \tag{66}$$

The time increment Δt^o may be interpreted as an average between the $\Delta t^{-\frac{1}{2}}$ and $\Delta t^{\frac{1}{2}}$. If we presume $\Delta t^{-\frac{1}{2}} = 0$, then $\Delta t^o = \Delta t^{\frac{1}{2}}/2$, i.e., half the initial time step. Thus

$$u_o^{\frac{1}{2}} \simeq 0.9091\text{x}10^{12} \; \Delta t^{\frac{1}{2}} \; (\text{cm/sec}) , \tag{67}$$

and the change in position of the boundary becomes

$$\delta R = u_o^{\frac{1}{2}} \Delta t^{\frac{1}{2}} \simeq 0.9091\text{x}10^{12} \; (\Delta t^{\frac{1}{2}})^2 \; (\text{cm}) . \tag{68}$$

If we ask that the initial change in the left-hand boundary be small compared to the zone size, say less than 10% of the first zone thickness, then

$$\Delta t^{\frac{1}{2}} < \sqrt{\frac{\Delta R}{0.9091 \times 10^{13}}} \simeq 0.33166 \times 10^{-6} \sqrt{\Delta R} . \qquad (69)$$

We are, then, led to an initial choice of time step of less than 0.33×10^{-6} sec. In this first example we have (arbitrarily) chosen to start with $\Delta t^{\frac{1}{2}} = 2 \times 10^{-7}$ sec, or, in the program units of milliseconds, $\Delta t^{\frac{1}{2}} = 2 \times 10^{-4}$ msec and $\Delta t^{0} = \Delta t^{\frac{1}{2}}/2 = 10^{-4}$ msec.

INTERPRETATION OF EXAMPLE PROBLEM NO. 1 OUTPUT

HAROLD TEST 1.* The problem is so labeled for Hydrodynamic And Radiation, One Lagrangian Dimension, and is preferred by some of us, as within the six letter limitation on notation. The senior author would prefer the short title RODHARD, standing for RAND One Dimensional Hydrodynamic And Radiation Diffusion, which is somewhat more descriptive.

IDEAL GAS. A further identification of the nature of the problem.

EQUATIONS OF STATE FOR THE GENERATOR. These equations of state are listed as a matter of record, since questions may otherwise arise at later times as to just what fits or tables were used. In this case, the Generator was provided with the two relations

$$P = (\gamma-1)E\rho \text{ as } FP1001 = .4*E/V, \qquad (70)$$

and

$$T = (\gamma-1)E/R \text{ as } FE1001 = .139*E. \qquad (71)$$

The Executor was given the single equation

$$P = .4*E/V, \qquad (72)$$

*Expressions in CAPITAL LETTERS or underscored are those appearing on the output sheets reproduced at the end of this section and to be explained or discussed here.

with the additional provision for temperature calculation at output times as specified in the Generator. For hydrodynamics, the temperature is not a sufficient nor a necessary quantity.

HISTORIES. To restart or continue the problem without beginning over again, tape histories can be provided periodically, storing data analogous to that necessary at the beginning and provided by the Generate subroutines. The selection of when such a tape record shall be written can be either by cycle intervals or by problem time intervals. Six successive rates may be specified. In this example, histories are called for every .025 milliseconds until 1 millisecond.

PRINTOUTS. The frequency at which specified listings of variables at all active mass zones will be listed can be similarly specified. In this case, we have elected to print out such data on the first three cycles to aid code checking. Subsequent listings of data are called for at cycle 10, at forty cycle intervals until cycle 263, at cycles 263 and 264 (to illustrate the variables just before and just after the combining of a pair of masses to accomodate an added zone), and at fifty cycle intervals thereafter until cycle 614.

ENERGY CHECKS. In many problems it is helpful to keep track of both the distribution of a net explosion energy and the total net energy, and this is provided in a print of the internal, kinetic and total energy in each region, as well as the sum of internal, kinetic and total energies over all the regions. In this example, since work is being done continuously by the pressure on the boundary, such an energy summation serves little purpose and little check on the accuracy of the calculation. Consequently, we have hoped to avoid any energy checks by selecting an interval larger than the expected length of the run (i.e., every 1000 cycles).

PMIN BNDRY COND. Whenever a special boundary condition is selected, it will be listed here. In this example, a constant pressure of 0.1 jerks*/meter^3 (1 kilobar) is applied at the lower (or left-hand) boundary - at j= -½ - for a very long time (for 10^{11} milliseconds).

RMIN = 1. This indication of the initial value of the position of the left-hand boundary is important in that it indicates a non-zero value of the position. Whenever the RMIN is started at exactly

*A jerk ≡ 10^{16} ergs.

zero value, the program avoids calculation of the velocity and the radius at that boundary, and consequently, the boundary remains at zero value throughout the problem. Such is the intention for spherical and cylindrical geometries, and could be the case where a rigid boundary is desired at the left of a plane geometry problem. In this case, both the velocity and the position at j=0 will be computed each cycle, and can be expected to change.

PLANE GEOMETRY. This is a reminder of the selected geometrical factor - that the problem is set up in plane rather than cylindrical or spherical symmetry.

REGION 1. MATERIAL 1001. Each region beginning at the left-hand boundary is designated with an increasing integer (region 1 being the first, region 2, next, etc.) and by a material number designation. The material number should correspond to one of those listed with the equations of state, and thereby identifies the material properties that will be ascribed to that region. Also listed for each region are the various selectable constants, C_1 through C_5. The definition of C_1 and C_2 is given in Eq. 13 or as the amplitudes selected for the quadratic and the linear terms of the artificial viscosity, respectively. Since the shock in this example will be a fairly strong one, no linear viscosity is necessary, and C_2 is set equal to zero. C_1 is chosen equal to 6. The number of zones to be expected in the shock front, as derived in a similar manner by von Neumann and Richtmyer[1] becomes

$$\text{Number of zones} \cong \pi\sqrt{2C_1/(\gamma+1)} \quad . \tag{73}$$

Since this example problem uses an ideal gas with $\gamma = 1.4$, a value of 6 for C_1 should build a shock spread of about 7 zones. If we were in water and so using a γ more nearly equal to 7, then a value of $C_1 = 14$ or 15 would be necessary to make a spread of six zones.

The Courant stability condition also includes an adjustable constant. As used in Eq. (36), C_3 represents a maximum value of γ, so in this case it can be taken as 1.4. It was in fact, taken as slightly larger, as 1.6, but that is not necessary.

The artificial viscosity stability condition involves a constant C4 which should be at least as large as four times C_1 (see Eqs. 47 and 50). Demonstrating a certain insensitivity in this condition, we have used without unstable results a value of only 16, while $4C_1 = 24$.

The radiation stability constant, C_5 (as defined in Section II) must be set to unity for explicit radiation diffusion. Larger values of C_5 are theoretically permissible for the implicit radiation formulation. For hydrodynamics, it is immaterial, and in this example, is set to zero.

The ambient energy for each region is also specified so that in totaling the energy of that region and/or of the whole system, the net energy introduced by a source (an explosive yield, or an influx of radiation energy) can be identified and maintained even as new zones (at ambient conditions) are added to the region. Since a continuous influx of energy is involved in this example problem, no attempt to account for the net energy will be made, and E = 0 will suffice. If one were to choose to include (or rather exclude) this ambient energy in the energy check sums, the appropriate value would be 0.2108, the same energy listed as initial value for the internal energy of the last zone.

The table of initial values which follows the list of constants specifies in the units of the code (the meter, millisecond, megagram system) for each zone the radius "R" (meters), particle velocity "U" (meters/millisecond), temperature "TEM" (10^4 °K), specific volume "VL" (m^3/megagram or cm^3/gm), pressure "PR" (jerks/m^3 = 10^{10} dynes/cm^2), and internal energy "EG" (jerks/megagram = 10^{10} ergs/gm). A vestige of code checking interests are the next two columns labeled "KP" and "KM". These are, respectively, the opacities at zone boundaries, using the density and the material designation (and so the opacity prescription) of the zone just ahead of the zone boundary $KP \equiv K_j(T_j, V_{j+\frac{1}{2}})$ and just behind the boundary $KM \equiv K_j(T_j, V_{j-\frac{1}{2}})$. Since this example does not include radiation, opacities are of no interest and have been left zero, as have luminosities in the last column labelled "EL".

The mass increments or elements are listed as "DMASS" in the next to the last column of the initial values table. The first column shows a spacing between zones of one centimeter (0.01 m) and the specific volume of 909.1 cm^3/gm corresponds to a density of $1.1x10^{-3}$ gm/cm^3 so that the mass elements, which in plane geometry are just the product of the zone dimension times the density, become $1.1x10^{-5}$.

Listed below the table of initial values are such factors as the initial time increments and others which have some arbitrariness of choice and so should be selected at the outset. The time increments during the problem running can be controlled automatically by the stability conditions, but the initial values must be chosen specifically. In this case, DT stands for the average of the current and just previous time increment (Δt^n) and is taken as half the current choice as if the previous value were zero. As discussed earlier, the value of the initial time step (DTP) has been chosen as $\Delta t^{n+\frac{1}{2}} = 2x10^{-4}$ msec.

If the problem involves the ingestion of mass or of new zones as it progresses, then some information must be supplied as to where zones are to be doubled and what size zones are to be added. Under MASS ADD INFO, J0 = 5 indicates that we have chosen to combine the fifth and sixth zones when new zones are needed (and then sequentially the next two zones, etc.). By JOS = 0 and JOM = 23 we have specified that when J0 has advanced to j = 23 it is to be set back to j = 0. The size of the added zones is given by DR. When DR is positive, it indicates directly the thickness of the added zone, such that in plane geometry $\Delta m=\rho\Delta R$, where ρ is the density of the last zone (at j=JMAX). When DR is given as a negative number, it indicates a fractional increment, as a fraction of the previous radius or the last position value (R_{jmax}), so that for this example, the first added zone will have a thickness $\Delta R = DR \cdot R_{30} = 0.0076923x1.3 = 0.01$ m.

The set of X's listed under PERCENTS are not percentages but are fractional numbers used in tests of the smallness of the change in computed quantities relative to the initial or final value of

that quantity. X1, X2, and X3 are associated with convergence routines in the radiation diffusion by implicit method, and are set to zero in this strictly hydrodynamic example. X4 = 0.4×10^{-5} indicates that a variable being determined in GETVAR has been found to be consistent with the determining values through the equation of state to a fractional accuracy of at least 4 parts in a million.

In problems where zones are added and combined automatically many times, there is the possibility of choosing J0, JOS, and JOM such that some region of the problem becomes too coarsely zoned. A check or control on the maximum size to which any one zone can grow is provided in the use of X5 since, before two zones are combined, their combined width is compared with X5 times the largest dimension or radius in the problem. In this case, the selection of X5 = 0.125 guarantees that no zone can become larger than one eighth of the largest radius. The last fraction, X6, is the convergence test for energy compatibility (in the energy conservation equation of the ROA routine) with pressure. Thus on successive evaluations, the internal energy shows a change of less than one part in ten thousand (for the value of X6 = 0.1×10^{-3}).

In this example, as often is the case, most of the zones in the problem are inactive initially, and need not be computed until some signal propagates into them. Since it is wasteful to compute through them, a floating boundary condition is set up which determines which will be the last zone to be calculated on each cycle. That last zone is denoted as "JHAT", which in this problem is started at 3. To advance JHAT when needed, a test is made on the temperature (if subroutine JHTT is used) or the particle velocity (if subroutine JHTU is used) at that last zone (j = JHAT) against a constant Z2. Whenever the temperature (or velocity) equals or exceeds Z2, JHAT is increased by unity, and one more zone is computed. In this example, we have chosen to test on velocity (using subroutine JHTU), and Z2 has been taken to be 10^{-4}.

The desired number of active zones is limited by the constant JL, such that whenever JHAT reaches JL, either another zone must be added while two other zones are combined (thus keeping JL constant), or a special boundary condition is applied, such as a free or fixed boundary.

The constant Z1 is similar to Z2 in that it determines the threshold temperature for adding another zone to the radiation diffusion part of a calculation. Since this example has no radiation flow, Z1 has been set to zero, but could have any value. Similarly, JSTAR, which denotes the last zone for radiation diffusion, has been chosen zero, but is of no consequence to this calculation.

The last cycle to be computed is denoted as NF, and is here chosen as 614.

A list of the subroutines used in the Executor follows the Generate input and starting data print-out.

The print-out for the actual execution of the problem begins with a title (TEST 1. HYDRO ONLY. IDEAL GAS), and then follows a list of the initial values of the selected variables displayed in the format chosen for those zones of index $J \leq JHAT + 3$. The units chosen for this test problem are the internal calculation units. The particular parameters chosen for output, and the order of output from left to right is zone number (j), radius, particle velocity, density, temperature, internal energy, pressure, artificial viscosity, and mass per zone. The artificial viscosity is a convenient indicator of compressions or shocks. The masses are constants of the motion in this Lagrangian system, but with the later periodic combining and adding of zones, its listing simplifies monitoring of zoning and makes any disparities in adjacent mass increments more readily identifiable.

Following the initial value listing is a line of information for the first cycle, a type of output which is presented for every cycle. Listed from left to right in the internal units of the program are the cycle number (n), the time at the end of the n-th cycle (milliseconds), the time increment for that cycle ($\Delta t^{n-\frac{1}{2}}$), LAMBDA (the maximum value of the artificial viscosity stability function), JLAM (the zone number of the largest value of LAMBDA), OMEGA (the normalized Courant stability conditions), JOMEGA (the zone number of the largest OMEGA value), GAMMA (the radiation diffusion stability control maximum value - not used in this pure hydrodynamics problem),

JGAM (the zone number of the most critical value of the radiation stability condition), JO (the next zone at which combining will take place), JSTAR (the largest zone through which radiation diffusion will be calculated, i.e., the outer boundary of the radiation diffusion - zero in this problem, since there is no radiation), JHAT (the last zone for which hydrodynamics will be calculated, i.e., the outer boundary), and IC (an iteration counter used in the implicit radiation routine - zero in this problem).

Outputs are listed for the first three cycles as an aid in code checking and to demonstrate the cycle-by-cycle progress of the finite difference method. Note that after the first cycle the kilobar boundary pressure (listed at j=0) causes some movement in the first (j=1) zone. This shows up as a non-zero velocity at the j=0 boundary and as an increase in density in the first zone. Corresponding increases in temperature, internal energy and pressure in that zone are also indicated, and because it is a compression, some artificial viscosity shows up.

On the second and third cycles, further growth of the movement is evident as the density continues to increase in the first zone and some compression reaches into the second zone. The very small and negative velocities that appear on the second and third cycles are a consequence of (and a measure of) the truncation error. Rounding the last figure of the pressures in adjacent zones slightly differently causes velocities of this small magnitude.

Note that the stability conditions have allowed the time increment to increase by 9/8ths on the second cycle, but have reduced Δt by 8/9ths <u>six</u> times to a value of $.98654 \times 10^{-4}$ on the third cycle to conform to the stability restriction from the growing artificial viscosity - indicating a growing shock in the first zone. The value of LAMBDA is near unity, while that of OMEGA is still quite small, indicating that the dominant stability is the viscosity or shock criterion (LAMBDA) rather than the Courant or sound speed condition (OMEGA).

By cycle 10, conditions in the first zone are well on their way toward representing a shock corresponding to the sudden onset of pressure we have exerted on the boundary. Between cycle 3 and 10 JHAT

has increased from 4 to 6 as more zones are set in motion. The density in the first zone is now nearly twice its original value.

By cycle 50, the shock is formed and is moving away from the boundary. Pressures, densities, temperatures, internal energies and velocities are all settling down to nearly constant values behind the front. At succeeding times (e.g., cycles 90, 130, 170, 210, and 250) all these quantities are within a percent or two of a constant value except for density, temperature, and internal energy in the first zone. The first zone or two are in this example somewhat anomalous, since they experienced a sudden onset of pressure - not a shock. The "definition" of a shock in such numerical schemes using artificially smeared fronts is one in which several zones of spread are necessary for normal propagation. When a boundary or initial condition prescribes a more rapid change or steeper gradients than are normally propagatable, the excessive heating of multiple or superimposed shocks is a natural consequence. Once a proper shock is developed, the appropriate Hugoniot values are generated.

The slight oscillations behind the shock cause small compressions and small artificial viscosity values. A linear viscosity term might be used to further damp such oscillations if desired. The last cycle run, cycle 614, has pressures as shown in Fig. 3 in comparison with the analytical exact solution (presuming a shock to have existed from the outset). The slight lag in the peak or shock front for the calculated pressure profile might have been eliminated by a set of initial conditions which more nearly represent the traveling shock including initial particle velocities as well as pressures in the first few zones and at the boundary itself.

The special display of cycles 263 and 264 allow a comparison of data just before and just after combining zones 5 and 6 into a single zone at 5. Note that on cycle 264 the mass at $j=5\frac{1}{2}$ (listed on line $j=6$) is the sum of the masses at lines 6 and 7 of cycle 263. The velocities, densities, energies, etc., are recomputed so as to conserve momentum and both kinetic and internal energy between the two zones and the new single zone. Mass conservation is automatic in the simple addition of masses. After combining, all the outer zones are shuffled

down to a zone number one less, and a new mass zone is added at the largest (right-most) zone boundary.

This simple test case problem takes about one minute for execution on the RAND machine combination 7040/7044 IBM.

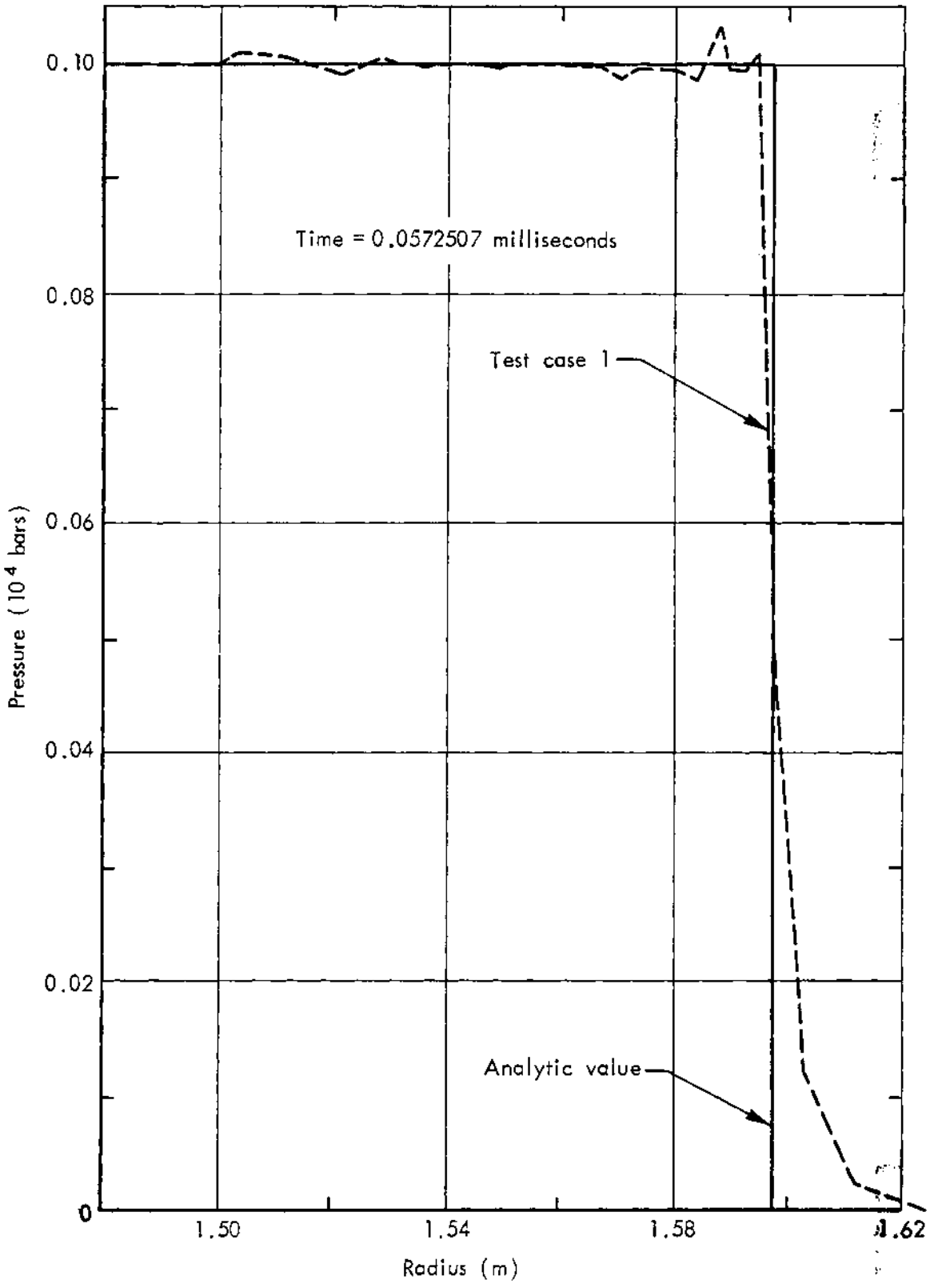

Fig.3—Calculated pressure profile compared with exact value

IV. RADIATION EXAMPLE

A somewhat more complex example may help to demonstrate the radiation aspects of the program. This second example will use spherical symmetry, radiation diffusion by the implicit formulation, single precision, analytic equations of state and opacities, two materials, grey-body radiation loss, and a different choice of output variables and units.

The physical situation chosen to demonstrate the interplay of radiation and hydrodynamics is that of air surrounding an aluminum sphere in which 10^{12} calories are released. This energy source is confined to the innermost one-fifth of the aluminum mass and is introduced uniformly in time over one-tenth of a microsecond. The mass of aluminum is taken as 100 pounds. Although this suddenly heated metal ball is not clearly a good model for an exploding nuclear device, it will serve well here to illustrate the essential features of the program in dealing with transient radiation flow problems where hydrodynamics also becomes important.

The air and the aluminum are characterized by analytic formulae for the equations of state and opacities and are presented in the listings at the end of this section. The analytic forms for air are particularly complex, and can lead to excessive running time for some problems, since the equations are computed through many hundreds of times for most cycles. The alternatives are to use simpler approximate fits (this one is good to 5% almost everywhere) or to use tabular forms. The formulae for aluminum used here are quite approximate but also fairly simple.

The CDR subroutine computes sources and sinks. In this example, it generates the initial energy (at a constant rate for a fixed time interval), and also calculates a grey-body radiation loss in the air which (by choosing an input option of IRAD=7 or 4) is computed using a special fit to the emissivity of air. A choice of IRAD=6 or 3 allows the subroutine to calculate this grey-body loss with the Rosseland mean free path of whatever material is exposed. This grey-body loss has the form

$$D = \sigma R^{(\delta-1)} T^4 (\Delta t)(\Delta R/\lambda)/(\Delta m), \qquad (74)$$

in which σ is the Stefan-Boltzman radiation constant, here equal to 5.67×10^{-4} jerks/meter^2/millisecond/10^4 degrees Kelvin, and λ is either the Rosseland mean free path or the emission mean free path for air. ΔR is the zone thickness, $R_j - R_{j-1}$ for the corresponding mass $\Delta m_{j-\frac{1}{2}}$. There is a further multiplicative factor when air is the outer region (IRAD = 4 or 7) which is an approximation to the cold air transmission cutoff in the ultraviolet (at 1860 Angstroms). In units of the code (temperature T in 10^4 degrees Kelvin) this factor is:

$$f = 25/(25 + 3.5 \times T^2 + T^3). \qquad (75)$$

The Generate print-out is similar to that for the first example, but now it is necessary to include a radiation stability constant. The implicit scheme in theory needs no limit on time step size, but some limit is necessary in practice both to avoid too many iterations per cycle and to avoid exceeding convergence domains which frequently seem to stem from the complexities of the equation of state fits. While the radiation front is building or when it is crossing a discontinuous boundary (between regions), it is prudent to limit the stability constant C5 to a value of about 1.5, but afterwards a much larger value is more economical. While too large a value necessitates too many iterations per cycle, too small a value restricts the size of the time increment without much reduction in number of iterations. The total number of passes through the iteration loop in advancing a given amount in problem time is a rough measure of running time economy, since the bulk of the computing, particularly with complex equations of state, is done in such loops (e.g., ROC, RDI, ROD loop).

The iteration procedure for convergence is arranged to become progressively less exacting as the number of iterations increases.

After five iterations the test on the fractional change of luminosities is dropped and only temperature changes are monitored for subsequent iterations. (See listing or flow diagram for the RDI subroutine.) After ten iterations, the fractional change of temperature is allowed to be four times larger (where initially $\delta T/T$ is tested against X3, now the test is against 4*X3). After 15 iterations the test is made against 20*X3, after 20 iterations against 100*X3, and after 25 times around the loop, the test on the iterative change in temperature relative to the temperature itself is that it be less than 1000*X3. At the twenty-fifth iteration a trouble-shooting print routine is activated, and most of the numerical values for parameters calculated in the relaxation loop are listed for all subsequent iterations until relaxation or until the 29th loop when the problem dies.

Settling for less accuracy when many iterations are required in finding a self-consistent set of temperatures and luminosities implies that the procedure is to some extent self correcting, and that subsequent cycles will not suffer from such a single or occasional reduction in accuracy. When a real instablity is in the making, such is not the case, but then, a cycle or two later, a stop is inevitable.

All of the test constants, X1 through X6, must be specified for this test case with radiation and with added zones. The X1 test occurs in the ROE subroutine in finding new temperatures in the hydrodynamic regions beyond the radiation diffusion region and is similar to the GETVAR routine which uses X4. Both X1 and X4 should be taken to have the smallest values (2×10^{-6}) of any of the test constants. Both require that temperatures derived for some value of energy and density will be correct (consistent) to two parts in a million. The X2 test occurs in the implicit iteration loop for luminosity convergence, and is taken here to be four times larger than X1 and X4. The X3 test determines the temperature convergence in the same implicit scheme, but is chosen here to have a value twice that of X1 or X4. The test of convergence in the first guess for temperatures and luminosities prior to entering the implicit iterative loop uses X6 and as such is allowed to be 100 times larger

than X1. The X5 constant controls the size of the doubled zones. If a pair of zones about to be merged into a single zone (CZR subroutine) promises to be thicker than X5 times the largest radius active in the problem (radius at JHAT), then that doubling is not allowed. With a value of 0.1, no zone will be allowed, through doubling of zones, to become larger than 10% of the maximum radius.

In the RAND version (but not the all-FORTRAN version), a set of variables and the units in which they will be presented are listed at the beginning of the output. The zero-cycle listing which follows shows the initial conditions to include no motion, normal 293 degree Kelvin (20°C) temperature, 14.63 psi ambient pressure in the air (something more than 2 kilobars in the aluminum initially), 1.2 kilograms per cubic meter air density, etc. INTENG stands for internal energy, DYNPRS for dynamic pressure ($\rho u^2/2$), ARTVIS for artificial viscosity, LMNSTY for luminosity, ROSMFP for Rosseland mean free path, NETPWR for net power as represented by the mean free path times the spacial gradient of luminosity ($\lambda\cdot(L_j-L_{j-1})/(R_j-R_{j-1})$), and RALORT for radiation loss rate as carried by half the THETA term or as $D*\Delta M$.

Note that on the first cycle, although the stability numbers are all small, convergence requires three iterations as indicated by iteration counter (IC).

Note that the energy check print-out after the first cycle shows some internal energy in the first region, indicating that the source term is active. The slight amount of kinetic energy in both regions stems from the small velocity that arises at the region interface (pressure in the aluminum being initially 35,360 psi).

The first cycle print-out shows the velocity at the interface, the corresponding dynamic pressures, the rise in the temperature, internal energy, and pressure in the first zone where the energy is being introduced as well as changes in luminosity, mean free path and net power. In the first zone, the radiation loss rate shows a negative value (-10^{19} cal/sec), which is the rate of input of source energy. Some slight radiation loss occurs at the interface also, but is unrealistic and negligible.

The next two cycles show the radiation flowing into the second zone as the source continues, and the energy increases. These consecutive cycle listings do not provide adequate data for easy code checking, since each cycle has several iteration loops within it. In the RDI subroutine, however, is a call for printing of much of the iterative loop function values, and it can be altered to print on every pass. (It is ordinarily set to print only after 25 iterations, to help in diagnosing a failure to converge.)

By the fourth cycle the number of iterations has risen to 7, but the stability conditions (LAMBDA, OMEGA, and GAMMA) are all less than unity, so the Δt is still allowed to increase. By the eleventh cycle, the radiation stability measure (GAMMA, with C5 = 1.5) has risen so that the next cycle must be at a smaller time increment. At this same time, the radiation has heated the fourth zone enough to include it in the radiation diffusion cycle (JSTAR increases from 3 to 4). As more and more energy is injected into the first zone, the temperatures rise, and the luminosities increase.

Although some compression is generated in the second zone by the high pressure in the first zone, and rather high velocities result (about 2000 ft/sec) in the first zone after the second cycle, the time is still too short for a change in the density to show up in the first four figures listed. On the first cycle print-out, small artificial viscosity pressures show up in all the aluminum zones. These are spurious, and are due to the slight difference in round-off between the densities as calculated in the generator and as computed here in the hydrodynamic subroutine (HYD). These viscosity terms in turn lead to the small velocities of cycle 2 for the same aluminum zones, although the first and last aluminum zones have larger velocities due to the pressure gradients between the heated first zones and the second zone and between the aluminum and air.

By the third cycle, slightly more than 5% of the energy has been injected, and it is still residing in the first zone of aluminum. The energy check sums (labeled E, K, W, Y, W-Y+Y) after cycle 3 show this clearly. They also show that no energy has been radiated from

aluminum to air or out of the air as yet (the Y terms being still negligible), nor has any net work been done on the air (W-Y+Y for region 2). The net work on region one is just the energy introduced into the aluminum.

By cycle 10, somewhat more than a third of the total energy to be introduced is now in the aluminum ("none" yet in the air). The time steps have been allowed to increase to nearly three times the original choice. However, the GAMMA term is growing rapidly as the radiation begins to flow, and by the 12th cycle it forces the Δt to decrease. A careful look at the output for cycle 10 will reveal the beginning of some rapid changes, for which smaller time steps are perhaps desirable. The innermost aluminum zone has a temperature of more than 15 million degrees, the velocity is more than 10^5 ft/sec, the densities are beginning to change, the pressure is high and the luminosity is rising. The Rosseland mean free path is larger, and the net power flux is approaching a few percent of the rate of introduction of energy. Essentially nothing is going on in the air, as yet.

By the thirtieth cycle, the time step (DT) has dropped again to what it started as. All the energy has just been put in by the source term, and on the next and succeeding cycles no more energy will be pumped into the first zone. Since the time did not quite reach 10^{-4} on the thirtieth cycle, but will exceed that value on the next cycle, not quite all the intended energy was introduced - lacking about ½%.* A little energy is now leaking out into the air by radiation diffusion (Y $\simeq$ 1.3%) and a little hydrodynamic work has been done on the air (W-Y+Y = 0.814342E-03). The outside of the aluminum sphere is just getting up to high velocity, and is still moving at about half of the velocity of the hot interior. None of the air is compressed, but the first air zone is already up to a tenth of a million degrees.

In the next thirty cycles the time advances to .159511 microseconds, and some eighteen percent of the energy flows into the air by radiation diffusion. This is shown by the energy check Y term for region 1 at cycle 60 (Y = .185566). Essentially all of this energy is in heat and shows as internal energy in air (E = 0.185538), with the corresponding kinetic energy for air (K = 0.0315925) being derived

*Recall that the source was chosen as a fixed rate ($\sim 10^{19}$ cal/sec for 10^{-7} sec), so that the exact energy could have been injected by fixing the time step or by calling for an output at that time.

from the work done by the expanding aluminum. The work term for air corresponds: W-Y+Y = 0.0315648.

The cycle 60 output shows that the aluminum temperatures have fallen, and the luminosities and mean free paths are also decreasing. At the same time, the velocities are increasing. The air is now hot out to about seven feet, and so a "fireball" has appeared.

At cycle 103 a special print occurs as directed by the GETVAR subroutine. Whenever the iteration count in the convergence loop which derives a temperature from a new internal energy exceeds 10, the print occurs, listing the zone number (16 in this case), the iteration count, the variables (OVAR and VAR, in this case since NV is 2, OVAR is the temperature and VAR is the specific volume), the function being worked with FN (in this case the energy, since MF = 2), and the desired final value for the function F.

When large changes in variables are taking place, the combined use of complicated equation of state functions and the Newton's Method may lead to trouble. The Newton's Method employs local slopes (derivatives) to approximate the change needed in the variable in order to arrive at the correct function value. Occasionally, as has happened here, a pair of points on the functional curve are struck such that the slopes from each return the variable to the previous value on the next step, i.e., the oscillation between two values is stable, and convergence is never achieved. To avoid such a needless catastrophe, the GETVAR subroutine kicks the convergence loop just once on the 16th iteration by taking the next guess as the average of the current and the previous guess. As is evident in this case, such a joggle can quickly lead to convergence.

The termination of the run at cycle 131 represents 10 minutes of execution. The next run was chosen to have C5 = 10, which allows a substantial increase in the time steps since the radiation diffusion stability (using C5) has been restricting the time steps. After regenerating with this change, the time steps increase (by 9/8ths) every cycle for twenty cycles, or by nearly an order of magnitude Δt (from .47E-05 at n=132 to .44E-04 at n=152).

The termination at cycle 197 represents another 10 minutes of running time. For the following run, C5 was increased to 20, but already the shock forming in the first zones of region 2 has raised the shock stability limit (LAMBDA) so that radiation limits as defined by C5 and GAMMA cease to restrict the time steps. GAMMA soon remains equal to ½ (its initial value when searching for the largest value) and Δt is reduced by the LAMBDA criterion as the shock continues to grow.

By the last cycle, (n=259) some 30% of the energy has diffused from region 1 into region 2, and a shock is beginning to grow at the outer edge of the radiation sphere in region 2 as well as from the rapid expansion at the inner edge. Carried to later times, the hydrodynamic expansion would soon dominate, and only slight radiative changes would be seen. Eventually, the grey-body radiation loss routine (CDR) would reduce the energy remaining behind the shock and lower the total net energy, but the radiation diffusion will all but cease, and could be eliminated at late stages without serious error. An appropriate choice of the critical temperature Z1 will keep JSTAR from growing beyond the hot region and will thus restrict the calculation of radiation diffusion to just those inner zones that remain hot after the shock passes.

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